SANDIA REPORT
SAND2007-42774277
Unlimited Release
Printed July 2007

Training Protocols for the Detection of Explosive Vapors in Interior Spaces

Stephen W. Webb and James M. Phelan

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia is a multiprogram laboratory operated by Sandia Corporation,
a Lockheed Martin Company, for the United States Department of Energy's
National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone:	(865) 576-8401
Facsimile:	(865) 576-5728
E-Mail:	reports@adonis.osti.gov
Online ordering:	http://www.osti.gov/bridge

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd.
Springfield, VA 22161

Telephone:	(800) 553-6847
Facsimile:	(703) 605-6900
E-Mail:	orders@ntis.fedworld.gov
Online order:	http://www.ntis.gov/help/ordermethods.asp?loc=7-4-0#online

SAND2007-42774277
Unlimited Release
Printed February 2007

Training Protocols for the Detection of Explosive Vapors in Interior Spaces

Stephen W. Webb
Geohydrology Department

James M. Phelan
Contraband Detection Department

Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-0735

Abstract

Computational fluid dynamics simulations for dispersal of explosive vapors in interior spaces have been performed including details of typical ventilation systems. The interior spaces investigated include an office area, a single-family house, and a warehouse store. Explosive vapor sources are defined in the various interior spaces, and contours of the vapor concentration in the interior spaces relative to the source concentration are presented for relative concentrations down to 10^{-5}. Training protocols for detection of explosive vapors in interior spaces should include an awareness of the time to equilibrium evident in these simulations as well as the significance of ventilation zones.

TABLE OF CONTENTS

LIST OF FIGURES

Training Protocols for the Detection of Explosive Vapors in Interior Spaces

Stephen W. Webb and James M. Phelan

1. Introduction

Explosive vapor emanations from target objects define an initial source release that is dependent on the external contamination and leakage rate of the explosive charge. Movement of the explosive vapors from the package into interior room volumes is influenced by the local environment, such as ventilation inflow and exhaust, thermal sources and air flow obstructions. With the emergence of small explosives vapor detection technology, operations teams need training on optimized search protocols that define best practices to determine the presence or absence of explosives in these locations. Computational fluid dynamics modeling can provide detailed estimates of the spatial and temporal vapor signatures available for detection that support definition of tactics and procedures for optimal use of explosives detection technology.

A series of room configurations containing target object placement have been developed. Simulation models for an office, a two-story residential house, and a warehouse store have been developed to cover a wide range of room sizes and configurations. These models include the appropriate ventilation system details, which are very important in distributing the explosive vapors throughout the domain. The FLUENT computational fluid dynamics code (Fluent, 2006) has been used to assess the temporal variation in spatial distribution/concentration of explosive signatures in these room configurations. The use of FLUENT for the dispersion of vapors in a room has been validated by comparison to experimental data (Chen and Srebric, 2001) for the release of sulfur hexafluoride (SF_6) in the office area model used in this study. Details of the data-model comparison show good agreement for the room air velocity, room temperature, and tracer gas dispersion.

For the purposes of these simulations, the tracer was modeled with TNT properties including a molecular weight of 227.13 g/mol and diffusivity in air of 6.4E-6 m^2/s. The source was defined as a surface with a constant gas mass fraction of 10^{-10}. Because TNT vapors have a tendency to sorb to most surfaces, the vapor was assumed to react completely and instantaneously with any surfaces in the model. The model results will thus show the lowest estimated vapor concentrations.

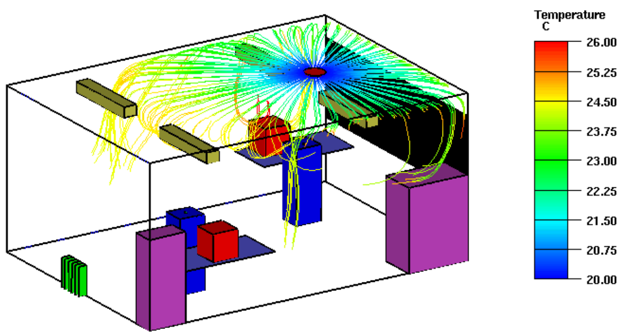
The model output that describes the movement of the explosive vapors is normalized to the defined source mass fraction for ease in comparing vapor dispersion results between room models and for extrapolation to other source emission assumptions. The model output concentration fractions need to be multiplied by the vapor concentration at the source to provide estimates for the absolute vapor concentration. This approach allows use of the same room dispersion results for alternate source mass fraction values, such as a much lower vapor pressure compound (e.g., RDX vapor pressure is ~ 1000x less than that of TNT) or a well sealed package that restricts source vapor emanations.

2. Results

The temporal variation in spatial distribution/concentration of explosive signatures in the various room configurations is given below for each individual room configuration in order of increasing size, starting with the office area, continuing onto the house, and finishing with the warehouse store.

A. Office Area

The office area (5.1 m length x 3.65 m height x 2.4 m width) consists of two human simulators, two desktops with computers, a window, two file cabinets, and overhead lighting fixtures mounted to the ceiling. The office is ventilated with a round ceiling diffuser that introduces air parallel to the ceiling, promoting mixing through the room, and returns through a low sidewall



vent on a wall at the end of the office.

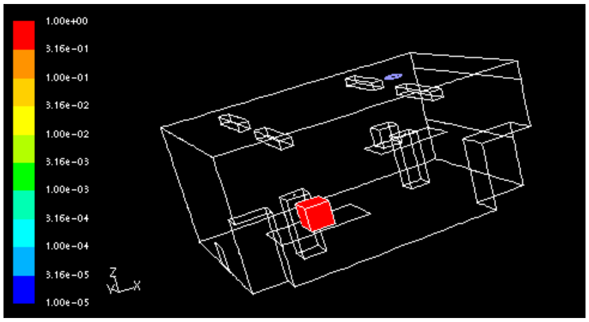
Figure 1. Office area showing pathlines of supply air colored by temperature

The ventilation system consists of

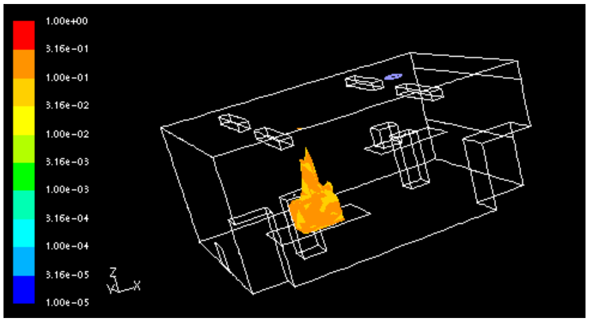
- One round ceiling diffuser (133. CFM @ 61^{o}F)
- One return vent (133. CFM)

The sensible heat from two (2) human simulators (150W or 75 W/person) is applied as a surface heat flux to the human simulator blocks. Light (136W or 34W each), energy from computers (108.5 W and 173.4 W), and external thermal boundary conditions (temperature profiles) for the walls and window have been applied. Turbulence and thermal radiation are included in the model.

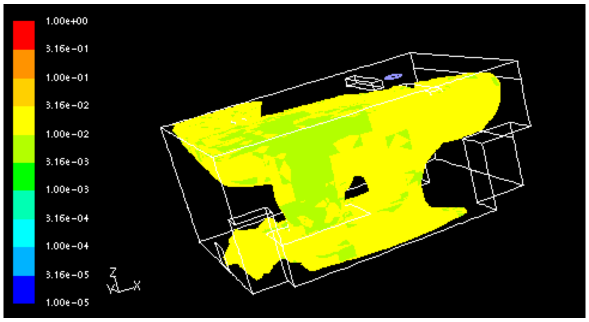
A constant concentration source emission was specified for one of the red boxes in Figure 1, which represents a computer monitor. The concentrations in the room reached steady-state values in about 5-10 minutes. After placement of the target object, chemical vapor emanations disperse with the local air movements and sorb to interior surfaces such that a constant spatial distribution of vapors was established in about 10 minutes. Because security search methods would not likely begin during the dynamic phase of the vapor dispersion in the room, only the steady-state values are shown.



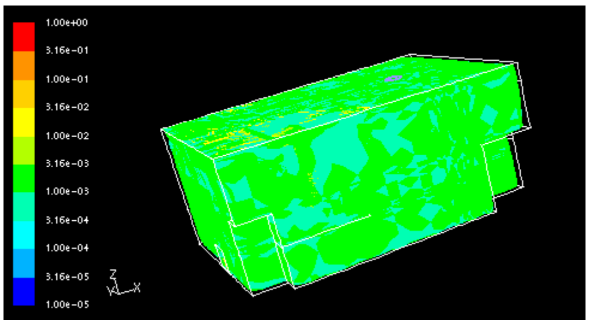
(a) Source Location (Relative Concentration = 1.0)



(b) Concentration Contours (Relative Concentration = 10^{-1})



(c) Concentration Contours (Relative Concentration = 10^{-2})



(d) Concentration Contours (Relative Concentration = 10^{-3})

Figure 2. Office Area Contours of Vapor Concentration Relative to Source Value

Figure 2 shows the concentration contours at various values relative to the source concentration over a three-order of magnitude range. Any finer resolution of the vapor concentration values does not improve the interpretive value. The concentration of vapors 10 times less than the source is found in the very near vicinity of the source. Because the vapor source is also a heat source, the vapors are driven upward by thermal lift as shown in Figure 2(b). At 10^3 times less than the source emission concentration, the room is entirely filled with dispersed vapors. Therefore, in order to quickly locate a room that may have a source, the detector must be capable of measuring vapors two to three orders of magnitude less than the source concentration. Using concentration gradients to locate the source may be difficult until the detector is placed in close proximity to the target.

B. Single-Family Home

This 3000 ft^2 two-story residential house (16 m length x 5 m height x 15 m width) consists of a playroom, living room, dining room, kitchen, study, foyer, and bath on the lower level and four bedrooms and two baths on the upper level. The HVAC system is comprised of two air conditioners with one in the basement serving the lower level and one in the attic serving the upper level. The ventilation supply grille diffusers are located in the floor of the lower level and in the ceiling of the upper level. The upper and lower levels are connected via a stairway in the foyer area.

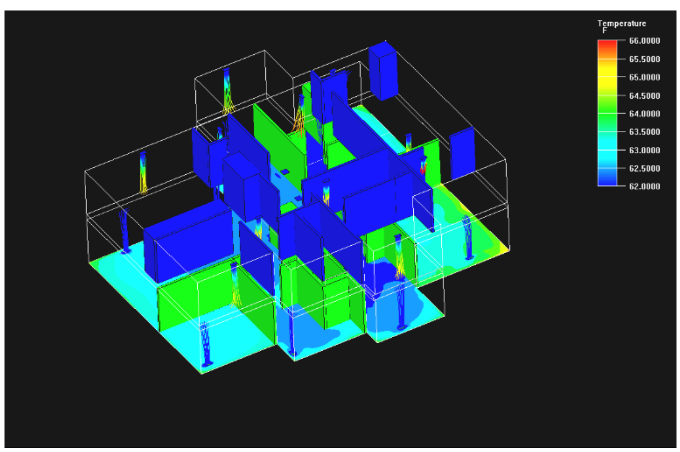


Figure 3. Single family home with mixing ventilation colored by temperature

The ventilation system consists of

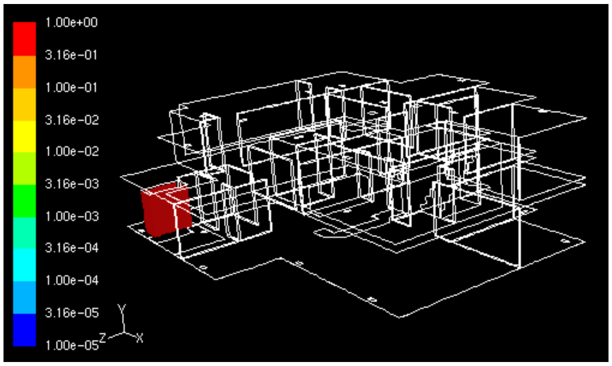
- Twenty-one (21) grille ventilation diffusers (25-115 CFM @ 60°F each)
- Six (6) return vents (250-480 CFM each)

Thermal boundary conditions (U-factor=0.3, external temperature =100°F) were applied to external walls. Turbulence and thermal radiation were included in the model.

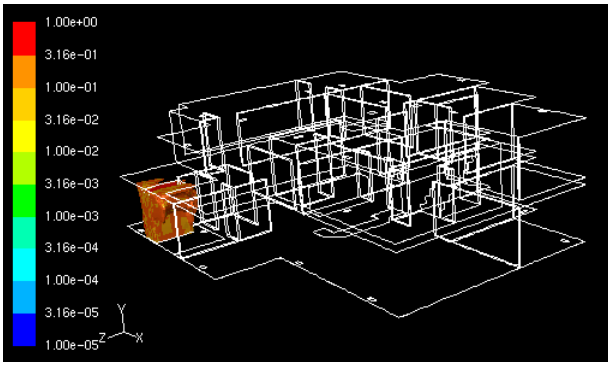
Dispersion results are provided for a source on the lower level and a source on the upper level.

1. Lower Level Source

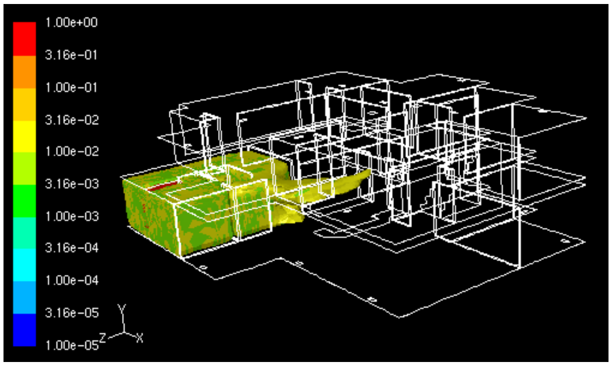
Figure 4 shows the concentration contours at various values relative to the source concentration over a five-order of magnitude range for a source on the lower level after 30 minutes. For this room and ventilation system configuration, the vapor concentrations on the lower level reach steady-state values in about 30 minutes. At longer times, there is some transport to the upper level, but these concentrations are very small and localized to the stairwell.



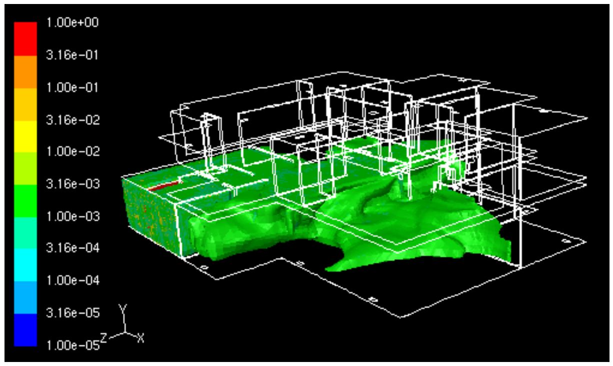
(a) Source Location (Relative Concentration = 1.0)



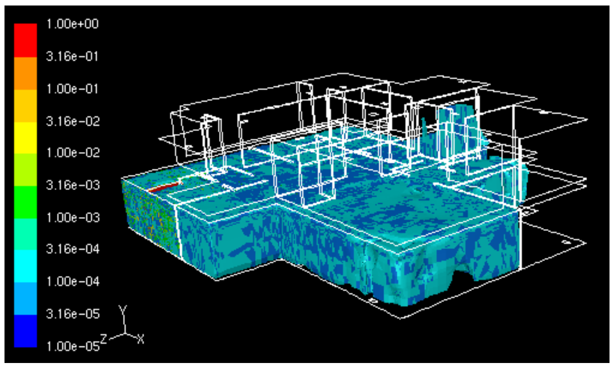
(b) Concentration Contours (Relative Concentration = 10^{-1})



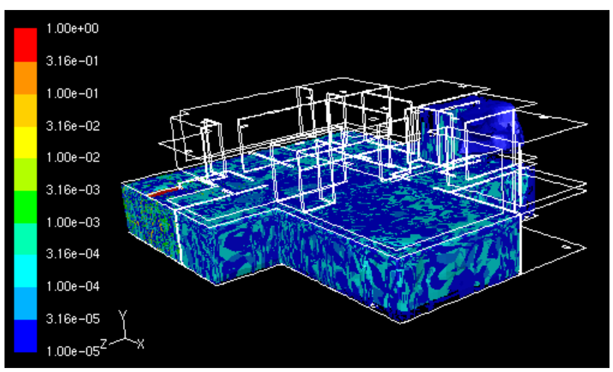
(c) Concentration Contours (Relative Concentration = 10^{-2})



(d) Concentration Contours (Relative Concentration = 10^{-3})



(e) Concentration Contours (Relative Concentration = 10^{-4})



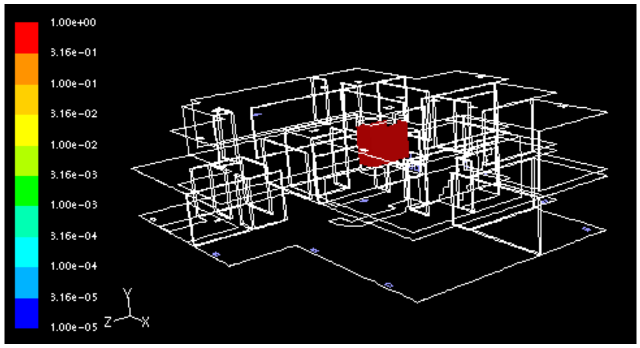
(f) Concentration Contours (Relative Concentration = 10^{-5})

Figure 4. Single Family Home Vapor Contours (lower level)

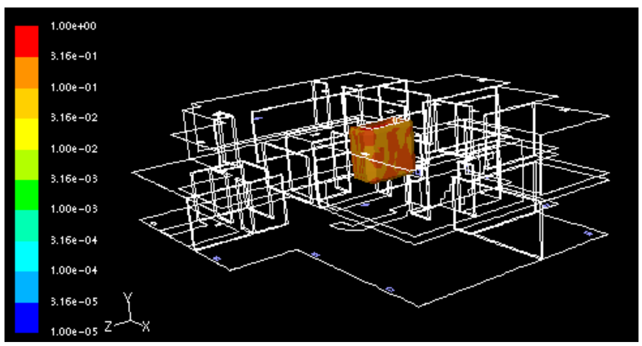
Just as in the office room configuration, the concentration drops off by one order of magnitude very close to the source (Figure 4(b)). In the vicinity of the room where the target is located, the vapor concentration is about 10^2 times less than the source (Figure 4(c)). Vapor concentrations at 10^3 times less than the source are found in adjacent rooms (Figure 4(d)). But, only when the vapor concentration is 10^4 times less than the source does the entire lower level show vapors fully dispersed throughout. At the lowest concentration contour, which is five orders of magnitude than the source, the vapor concentration begins to show on the upper level (Figure 4(f)).

2. Upper Level Source

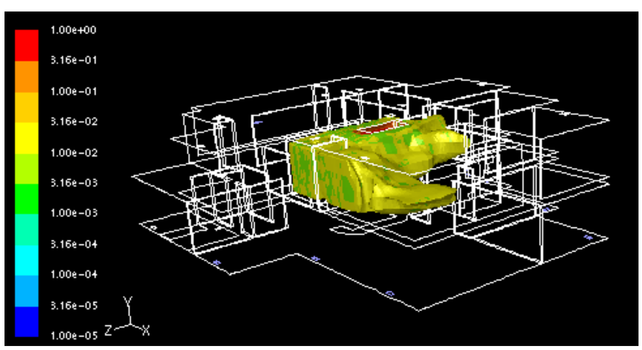
Figure 5 shows the concentration contours at various values relative to the source concentration over a five-order of magnitude range for a source on the upper level. The vapor concentrations on the lower level reach steady-state values in about 60 minutes. At longer times, there is some transport to the lower level, but these concentrations are very small and localized to the stairwell.



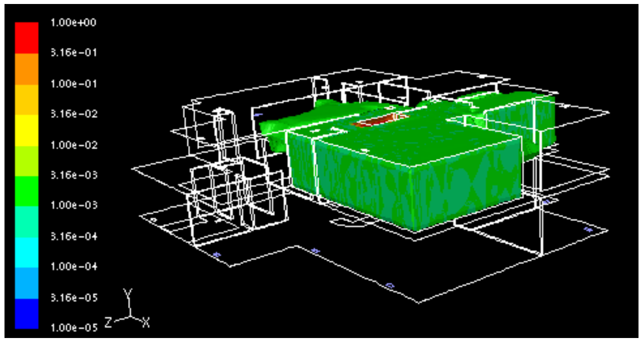
(a) Source Location (Relative Concentration = 1.0)



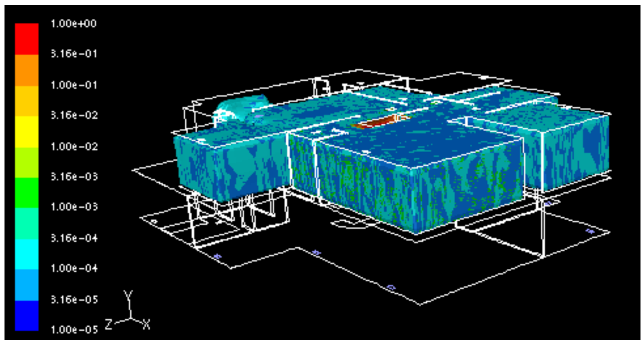
(b) Concentration Contours (Relative Concentration = 10^{-1})



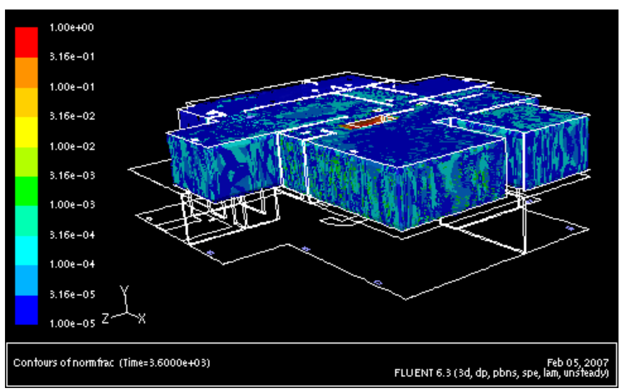
(c) Concentration Contours (Relative Concentration = 10^{-2})



(d) Concentration Contours (Relative Concentration = 10^{-3})



(e) Concentration Contours (Relative Concentration = 10^{-4})



(f) Concentration Contours (Relative Concentration = 10^{-5})

Figure 5. Single Family Home Vapor Contours (upper level)

These results are very similar to the source on the lower level. The concentration drops off by 10 fold very close to the source (Figure 5(b)). In the vicinity of the room that contains the target, the vapor concentration is about 10^2 times less than that of the source (Figure 5(c)). At 10^3 times less than the source, adjacent rooms show the presence of dispersed source vapors (Figure 5(d)). The entire upper level shows vapors with concentrations about 10^4 times less than the source. At the lowest concentration level, which is five orders of magnitude than the source, the vapor concentration from a source on the upper level is fully dispersed throughout the upper level, and begins to be found on the lower level.

C. Warehouse Store

This warehouse store (137 m length x 9 m height x 55 m width) is representative of many which are populating America today (Figure 6). The store consists of many aisles that allow customers to walk through shelved areas displaying products. The store is ventilated by many diffusers located on ducts near the ceiling with many returns also located near the ceiling. This is a mixing-type ventilation system that is designed to produce comfort conditions and maintain acceptable air velocities in the lower occupied regions of the store. This particular model contains virtual air handling units (AHUs) which exchange outside air (OA) for some of the return air and cool the mixed air before supplying the air back to store through the supply diffusers. The outside air exchange provides for greater dilution of source vapors than for room configurations without outside air exchange.

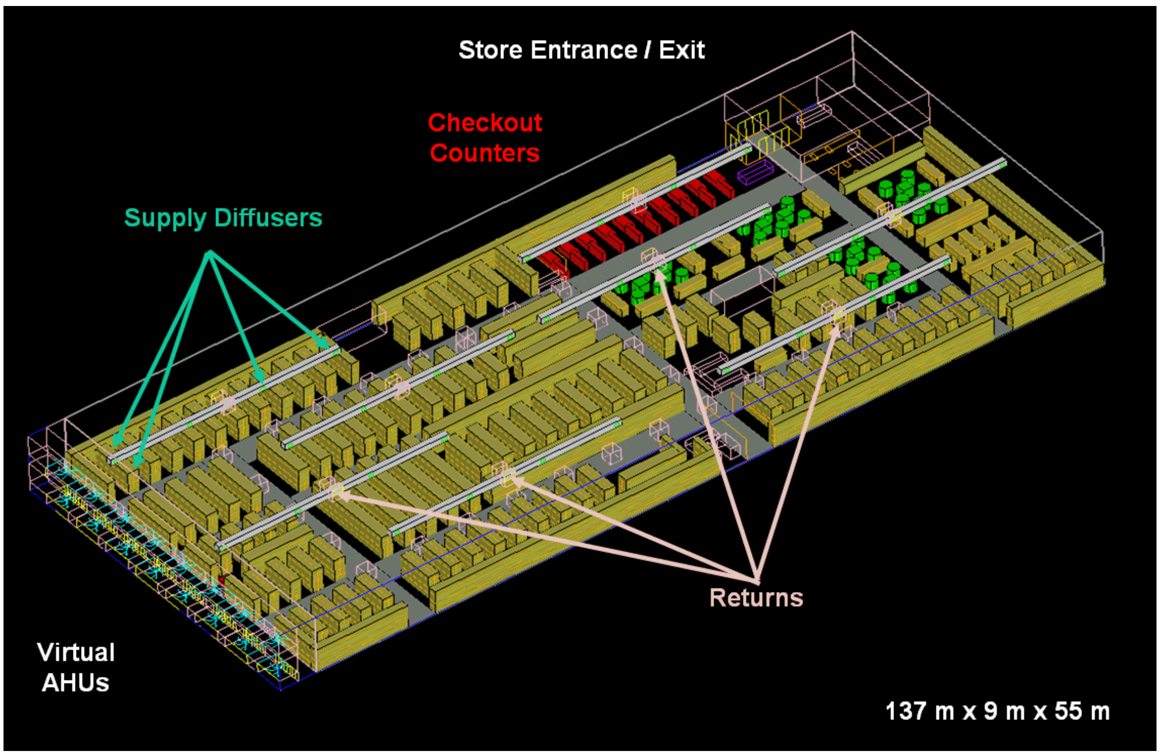


Figure 6. Layout of warehouse store

The ventilation system consisted of

- Eight air handling units (AHUs)
    - Eight supply diffusers per AHU set to deliver 4,900 CFM @ 65°F each.
    - One return grille per AHU set to return 39,200 CFM
    - For each AHU, 1562.5 CFM (based on 20 CFM per occupant) of outside air introduced @ 90°F, 30% RH.

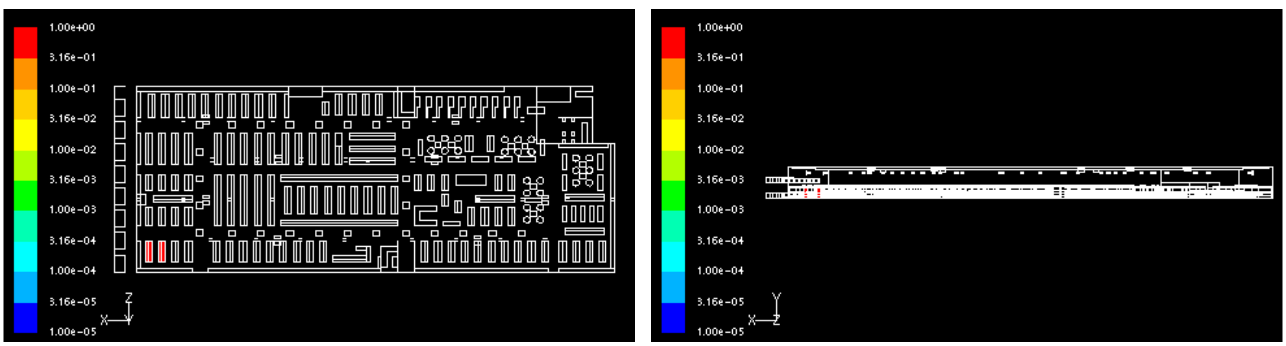
Thermal boundary conditions for the analyses include the sensible heat from approximately 625 people in the store (100 kW or about 160 W/person), lighting (200 kW or 30 W/m^2), and wall boundary conditions

- North wall – U factor = 1 W/m^2K, external temperature = 90° F, convection
- South wall – U factor = 1 W/m^2K, external temperature = 118°F, solar radiation and convection.
- East wall – U factor = 1 W/m^2K, external temperature = 115°F, solar radiation and convection
- West wall – U factor = 1 W/m^2K, external temperature (conditioned space) = 75°F, convection

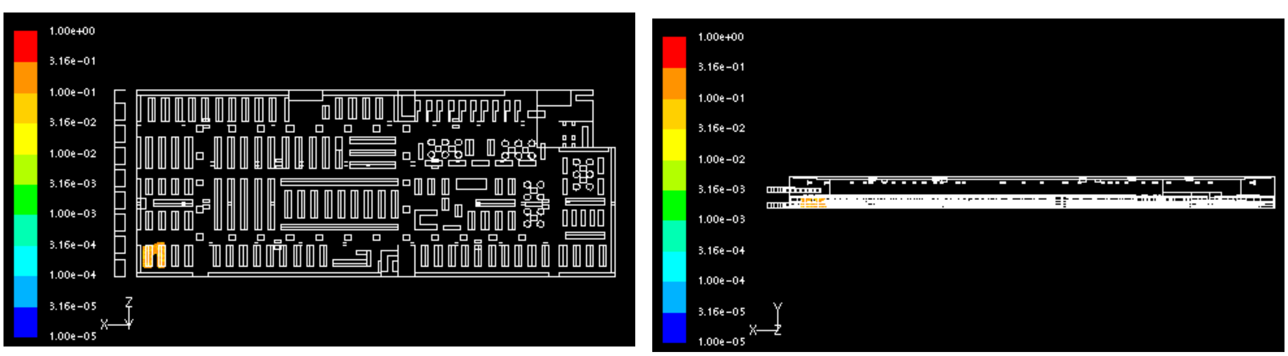
- Adiabatic conditions on all other walls

Turbulence and thermal radiation are included. The source is located in the lower left part of the store.

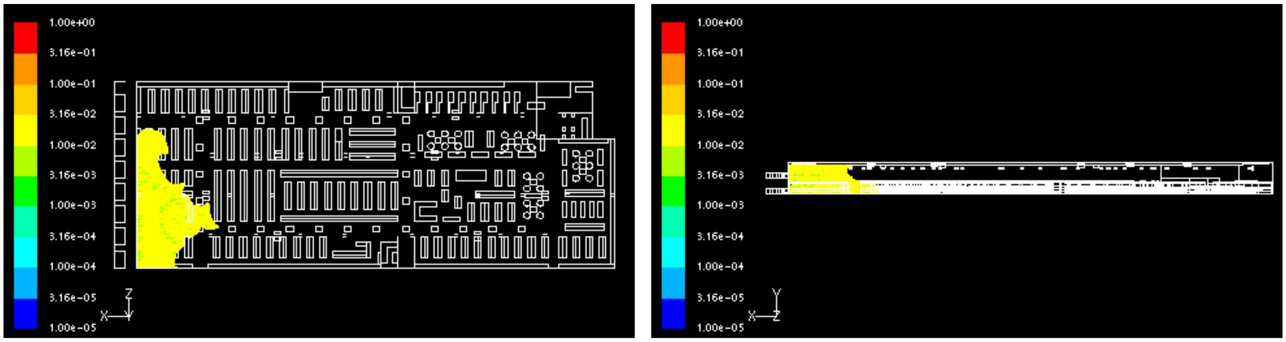
Figure 7 shows the concentration contours at various values relative to the source concentration over a five-order of magnitude range. Both horizontal and vertical cross sections are shown. Note that there is an open exit in the upper right corner in the plan view of the warehouse. The vapor concentrations reach steady-state values in about 10 minutes or less due to the large ventilation rate.



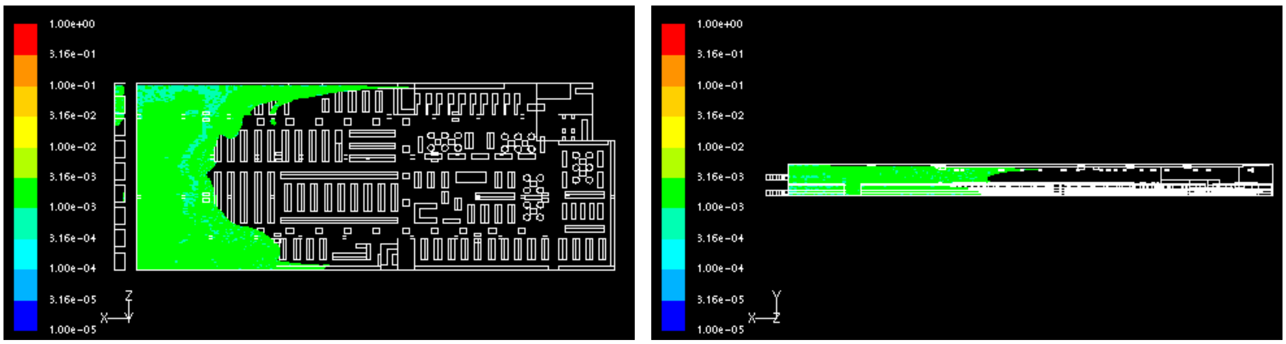
(a) Source Location (Relative Concentration = 1.0)



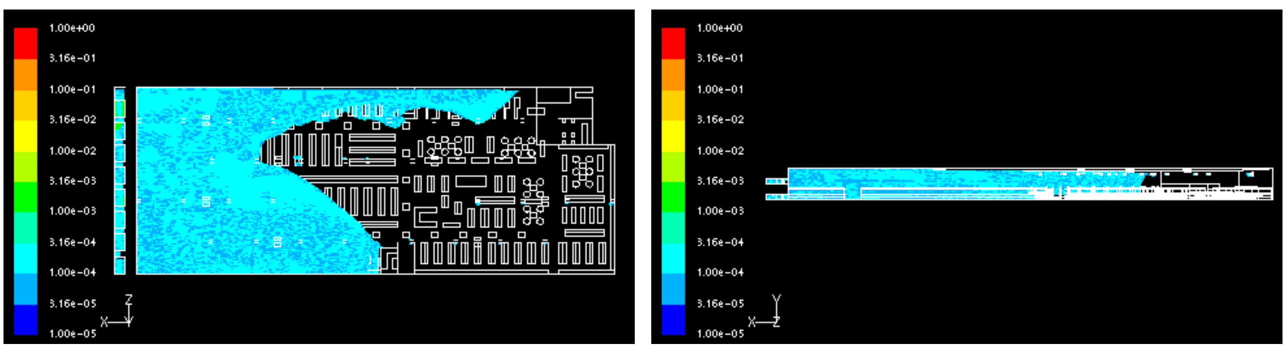
(b) Concentration Contours (Relative Concentration = 10^{-1})



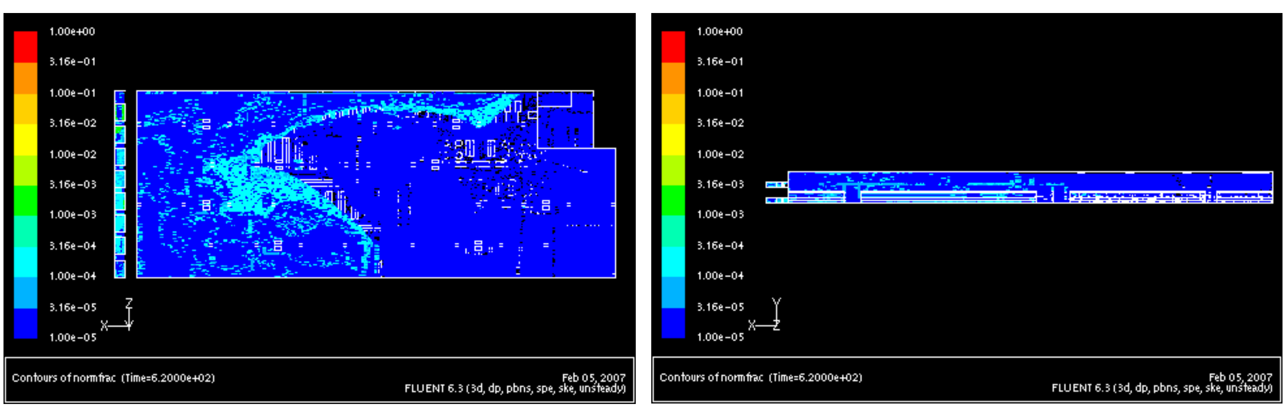
(c) Concentration Contours (Relative Concentration = 10^{-2})



(d) Concentration Contours (Relative Concentration = 10^{-3})



(e) Concentration Contours (Relative Concentration = 10^{-4})



(f) Concentration Contours (Relative Concentration = 10^{-5})

Figure 7. Warehouse Room Vapor Contours

3. Discussion

Computational fluid dynamics simulations for dispersal of explosive vapors in interior spaces have been performed including details of typical ventilation systems. The interior spaces investigated include an office area, a single-family house with separate lower and upper level sources, and a warehouse store. Based on the results of this study, the time to the equilibrium vapor concentration is quite rapid, typically less than 1 hour for all three simulated scenarios. This time depends on the capacity and operational characteristics of the ventilation system of the various room configurations.

For all three room types, a similar pattern of vapor dispersion contours is evident. Decade difference contour plots showed the vapor dispersion distance from the source and coverage within various zones of the domain. The locations containing vapor concentrations 10 times less than the source were all in close proximity to the source (within a few feet or less). The locations containing vapor concentrations 10^2 times less than the source were typically found in the same room (office and home) or within a couple of aisles in the warehouse store. The locations with 10^3, 10^4 and 10^5 fold reduced vapor concentrations were found in increasing larger zones, inclusive of the ventilation inflow and return paths. In the office, this zone of ventilation is the entire room. In the house, the upper and lower levels are separate zones of ventilation. In the warehouse store, the entire store is a zone of ventilation. It is important to understand ventilation zone(s) in any building to be searched for explosive vapors as the vapors will generally stay within the originating ventilation zone.

Training protocols for detection of explosive vapors in interior spaces should include an awareness of the time to equilibrium evident in these simulations as well as the significance of ventilation zones.

4. Conclusions

Based on the results of this study, the behavior of explosive vapors is as follows:

1. Time to equilibrium vapor concentrations in the interior spaces is quite rapid, typically less than 1 hour.

2. Vapor concentrations decrease rapidly from the source value, typically decreasing by an order of magnitude within a few feet of the source, and two orders of magnitude within the same room in an office or house or a couple of aisles in a warehouse store.

3. The ventilation zone(s) within a building or interior space need to be understood. The vapors generally stay within the originating ventilation zone.

Training protocols for detection of explosive vapors in interior spaces should include an awareness of the time to equilibrium evident in these simulations as well as the significance of ventilation zones.

5. References

Chen, Q. and J. Srebric, 2001, "Simplified Diffuser Boundary Conditions for Numerical Room Airflow Models," ASHRAE RP-1009.

Fluent, Inc., 2006, FLUENT 6.3 User's Guide, Fluent, Inc., Lebanon, NH, September 2006.

Distribution

5	MS0735	S.W. Webb, 6313
5	MS0782	J.M. Phelan, 6418
1	MS1168	C.A. Hall, 1646
1	MS1455	C.A. Gresham, 2555
1	MS0782	K.L. Linker, 6418
1	MS1133	S.N. Todd, 5916
2	MS9018	Central Technical Files, 8944
2	MS0899	Technical Library, 04535